Optimum Phase Space Probabilities From Quantum Tomography

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We determine a positive normalised phase space probability distribution P with minimum mean square fractional deviation from the Wigner distribution W .The minimum deviation, an invariant under phase space rotations, is a quantitative measure of the quantumness of the state.The positive distribution closest to W will be useful in quantum mechanics and in time frequency analysis .

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1. Quasi-probability distributions in Quantum Mechanics and Time Frequency Analysis.

The Wigner quasi-probability distribution W [1],first proposed to calculate quantum corrections to thermodynamic equilibrium, is now widely used in quantum mechanics, statistical mechanics, and technological areas such as time-frequency analysis of signals in electrical engineering and seismology [2]. The W distribution and other quasi-probability distributions such as the Husimi Q function [3] ,the Glauber-Sudarshan P function and their s-parametrized generalizations [4] can be obtained in quantum optics by measuring probability distributions of quadrature phases and making an inverse Radon transform, i.e. quantum tomography [5]. The Wigner function has the unique distinction of being the quantum analogue of the classical Liouville phase space distribution since its marginals reproduce quantum probability densities of position coordinates q_i, momentum coordinates p_i and indeed of quadrature phases $q_i \cos\theta_i + p_i \sin\theta_i$ for all θ_i with i taking N values for a $2N$-dimensional phase space.In time frequency analysis too W has the correct marginals reproducing energy densities in time or frequency.

Unlike the classical Liouville density, W cannot be interpreted as a joint probability density, because there are quantum states for which W is not positive definite. Similarly in time-frequency analysis W, has marginals reproducing the energy densities in time or frequency but cannot be interpreted as their joint density ; for that one uses the positive definite 'Spectrogram' even though it does not have the correct marginals. In quantum mechanics, the main reason for the importance of the Husimi function Q (a smeared W function) is that it is positive definite ; secondly,as shown by Braunstein, Caves and Milburn, it is the optimum of the distributions obtained in the Von-Neumann-Arthurs-Kelly model for joint measurement of position and momentum [3]. However, its marginals differ from the corresponding quantum probability densities, even when the W function is positive definite. This motivates the variational problem seeking the best possible positive distribution.The positive joint probability we find has immediate utility for quantum mechanics (especially quantum optics) and in time-frequency analysis with obvious transcriptions of the variables (q, p going to t, ω) as improvement over the Husimi Q function and the Spectrogram $P_{SP}(t,\omega)$ respectively.

2. Positive joint probability distribution closest to the Wigner distribution and a measure of quantumness. Suppose we know W through quantum tomography. We seek a criterion invariant under phase space rotations to define the positive definite phase space probability density 'closest' to the W function and with total phase space integral unity, as necessary for a probability interpretation. The criterion of 'closeness' must be such that it gives back the W function when that is positive definite. In $2N$ dimensional phase space, with units $\hbar = c = 1$, the Wigner function is given in terms of the density operator ρ ,

$$W(\vec{q},\vec{p}) = \frac{1}{(2\pi)^N}\int d\vec{y}\exp(i\vec{p}.\vec{y})\langle\vec{q}-\vec{y}/2|\rho|\vec{q}+\vec{y}/2\rangle$$
$$= \frac{1}{(2\pi)^{2N}}\int d\vec{\xi}\int d\vec{\eta}\, Tr\rho\exp(i\vec{\xi}.(\vec{q}_{op}-\vec{q}) + i\vec{\eta}.(\vec{p}_{op}-\vec{p})), \quad (1)$$

where time dependence of the density operator and the Wigner function have been suppressed, $\vec{q}_{op}, \vec{p}_{op}$ denote the position and momentum operators and the last equation facilitates discussion of rotation properties in phase space.In quantum optics,

$$\vec{q}_{op} = (\vec{a}+\vec{a}^\dagger)/\sqrt{2},\ \vec{p}_{op} = -i(\vec{a}-\vec{a}^\dagger)/\sqrt{2}. \quad (2)$$

We vary $P(\vec{q},\vec{p})$ so as to minimise,

$$\sigma^2 = \frac{\int d\vec{q}\int d\vec{p}\,(P(\vec{q},\vec{p}) - W(\vec{q},\vec{p}))^2}{\int d\vec{q}\int d\vec{p}\,W(\vec{q},\vec{p})^2} \quad (3)$$

(which is just the mean of the square of the fractional deviation $(P-W)/W$ with the weight function W^2), subject to the constraints,

$$\int d\vec{q}\int d\vec{p}\,P(\vec{q},\vec{p}) = 1;\ P(\vec{q},\vec{p}) \geq 0. \quad (4)$$

We use Lagrange's method of undetermined multipliers modified to incorporate inequality constraints. The above normalization constraint is equivalent to

$$\int d\vec{q}\int d\vec{p}\,(P(\vec{q},\vec{p})-W(\vec{q},\vec{p}))=0, \quad (5)$$

and the expression for σ^2, using Moyal's well known result for phase space integral of W^2 [1] simplifies to

$$\sigma^2=(2\pi)^N\int d\vec{q}\int d\vec{p}\,(P(\vec{q},\vec{p})-W(\vec{q},\vec{p}))^2. \quad (6)$$

This leads to the Lagrangian,

$$\begin{aligned} L=&\int d\vec{q}\int d\vec{p}\,(P(\vec{q},\vec{p})-W(\vec{q},\vec{p}))^2\\ &+2c\int d\vec{q}\int d\vec{p}\,(P(\vec{q},\vec{p})-W(\vec{q},\vec{p})), \end{aligned} \quad (7)$$

where c is the Lagrange multiplier. Following a method used widely by Martin to incorporate inequality constraints [6], we prove by direct subtraction that σ^2 has a global minimum when we choose $P(\vec{q},\vec{p})=P_{min}(\vec{q},\vec{p})$, where,

$$P_{min}(\vec{q},\vec{p})=P_0(\vec{q},\vec{p})\,\theta(P_0(\vec{q},\vec{p})), \quad (8)$$

where $\theta(x)$ is the Heaviside θ function, being unity when the argument is positive and zero otherwise, and

$$P_0(\vec{q},\vec{p})=W(\vec{q},\vec{p})-c. \quad (9)$$

Denoting by L and L_{min} respectively the values of the Lagrangian for an arbitrary $P(\vec{q},\vec{p})$ satisfying the constraints, and by $P_{min}(\vec{q},\vec{p})$, we obtain,

$$\begin{aligned} L-L_{min}=&\int_{P_0\geq 0}(P-P_0)^2 d\vec{q}d\vec{p}\\ &+\int_{P_0\leq 0}(P^2-2PP_0)d\vec{q}d\vec{p}\geq 0, \end{aligned} \quad (10)$$

since each of the two integrands is non-negative. We complete the proof by showing the existence and uniqueness of a constant c satisfying the normalization constraint,

$$\int_{W(\vec{q},\vec{p})-c\geq 0}(W(\vec{q},\vec{p})-c)d\vec{q}d\vec{p}=1. \quad (11)$$

First, if W is non-negative, $c=0$ is the unique solution, and gives $\sigma^2=0$. Suppose now that W is negative in some regions of phase space. The left-hand side integral is then ≥ 1 for $c\leq 0$, decreases monotonically as c increases to positive values until it equals 0 when $c=max_{\vec{q},\vec{p}}W(\vec{q},\vec{p})$. Hence there is a unique solution for c in the interval $[0,max_{\vec{q},\vec{p}}W(\vec{q},\vec{p})]$. Using this value of c we compute the optimum phase space probability distribution as well as the minimum value of σ^2, an index of quantumness of the state .

3. Incorporating additional rotationally invariant constraints in phase space . In addition to the phase space volume, the surface of the sphere with centre $\vec{q}_{cl},\vec{p}_{cl}$

$$(\vec{q}-\vec{q}_{cl})^2+(\vec{p}-\vec{p}_{cl})^2=x$$

is an invariant under rotations in phase space ; the expectation value of the left-hand side given by the Wigner function agrees with the quantum result and hence may be used as an additional constraint. Further, if W remains positive in the region $x\geq x_{max}$, we may choose $P(\vec{q},\vec{p})=W(\vec{q},\vec{p})$ in that region, and for sufficiently large x_{max} ,still find a solution $P(\vec{q},\vec{p})$ that minimises σ^2 under the positivity constraint $P(\vec{q},\vec{p})\geq 0$, the normalisation constraint,

$$\int\int_{x\leq x_{max}} d\vec{q}d\vec{p}\,(P(\vec{q},\vec{p})-W(\vec{q},\vec{p}))=0, \quad (12)$$

and the additional constraint,

$$\int\int_{x\leq x_{max}} d\vec{q}d\vec{p}\,(P(\vec{q},\vec{p})-W(\vec{q},\vec{p}))x=0. \quad (13)$$

If we choose $\vec{q}_{cl},\vec{p}_{cl}$ as the quantum expectation values of $\vec{q}_{op},\vec{p}_{op}$, the last equation imposes the sum of quantum dispersions $(\Delta\vec{q})^2+(\Delta\vec{p})^2$ as a constraint. We then prove as before that the solution minimising σ^2 is, for $x\leq x_{max}$

$$P_{min1}(\vec{q},\vec{p})=P_{01}(\vec{q},\vec{p})\,\theta(P_{01}(\vec{q},\vec{p})), \quad (14)$$

where

$$P_{01}(\vec{q},\vec{p})=W(\vec{q},\vec{p})-c-xd, \quad (15)$$

provided that constants c,d are found satisfying the two equality constraints given above.

4. Optimum positive joint probability distributions and Husimi distribution for generalized coherent states . The Husimi Q function in $2N$-dimensional phase space is,

$$Q(\vec{q},\vec{p})=(2\pi)^{-N}\langle\vec{\alpha}|\rho|\vec{\alpha}\rangle \quad (16)$$

where $|\alpha\rangle$ are the coherent states,

$$\vec{a}|\vec{\alpha}\rangle=\vec{\alpha}|\vec{\alpha}\rangle\,,\vec{\alpha}=(\vec{q}+i\vec{p})/\sqrt{2}.,, \quad (17)$$

Generalized coherent states [7] are displaced excited eigen state solutions of the time dependent Schrödinger equation for the one dimensional oscillator whose probability density packets move classically with shape unchanged, and have uncertainty product $\Delta q\Delta p=n+1/2$,

$$\begin{aligned} \langle q|\psi(t)\rangle=&\langle q-q_{cl}(\tau)|n\rangle\exp(-i(n+1/2)\tau)\\ &\exp(i\dot{q}_{cl}(\tau)(q-1/2\dot{q}_{cl}(\tau))), \end{aligned} \quad (18)$$

where, $|n\rangle$ is the n-th excited state and q_{cl} has classical motion

$$\tau=\omega t,\ q_{cl}(\tau)=A\cos(\tau+\phi). \quad (19)$$

The quantum expectation values for position and momentum operators are,

$$\langle q_{op} \rangle = q_{cl}(\tau),\ \langle p_{op} \rangle = \dot{q}_{cl}(\tau) \equiv p_{cl}. \tag{20}$$

Wigner functions and Husimi functions can be seen to depend on q, p only through the combination,

$$x = (q - q_{cl})^2 + (p - p_{cl})^2. \tag{21}$$

For $n = 0$ the optimum phase space probability density is just the Wigner function which is positive definite. For $n = 1, 2$ the $W_n(q,p)$ and $Q_n(q,p)$ functions are given by,

$$W_1 = (2/\pi)(x - 1/2)\exp(-x),$$
$$Q_1 = (x/(4\pi))\exp(-x/2), \tag{22}$$

$$W_2 = (2/\pi)((x-1)^2 - 1/2)\exp(-x),$$
$$Q_2 = (x^2/(16\pi))\exp(-x/2). \tag{23}$$

We have numerically evaluated the optimum phase space probability distributions P_{min}, P_{min1}. With P_{min}, for $n = 1, c = .0105338, \Delta q \Delta p = 1.10753, \sigma^2 = .277049$; for $n = 2, c = .0159546, \Delta q \Delta p = 1.72182, \sigma^2 = .268084$. With P_{min1} ,for $n = 1, x_{max} = 18, c = .0183706, d = -.00141308, \sigma^2 = .287684$; for $n = 2, x_{max} = 15, c = .0423479, d = -.00408366, \sigma^2 = .322254$. With the Husimi distribution, for $n = 1, \Delta q \Delta p = 2, \sigma^2 = .509259$; for $n = 2, \Delta q \Delta p = 3, \sigma^2 = .64429$. We compared the optimum P_{min}, P_{min1} with W, Q distributions in Figs. 1,2. We also compared the corresponding position probability densities in Figs. 3,4. The improvement over the Husimi function is obvious qualitatively from the figures, and quantitatively from the σ^2 values.

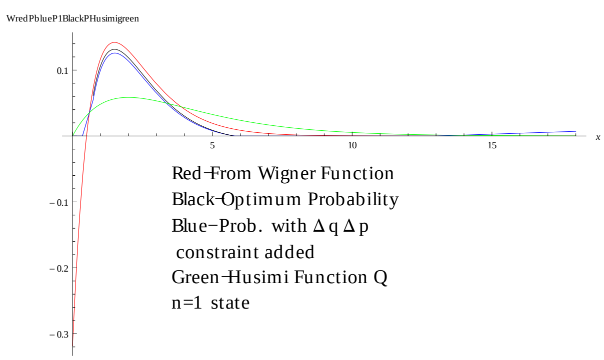

FIG. 1: For the n=1 coherent state , the optimum phase space probability distributions with only normalization constraint, and including additional constraints fixing $\Delta q \Delta p$ are compared with the Wigner and Husimi distributions as a function of $x = (q - q_{cl})^2 + (p - p_{cl})^2$. The optimum and Husimi distributions have $\sigma^2 = 0.277049$, and 0.509259 respectively.

5. Optimum Positive Phase Space Densities Reproducing $N + 1$ Quantum Marginals . Cohen and Zaparovanny [8] constructed the most general positive

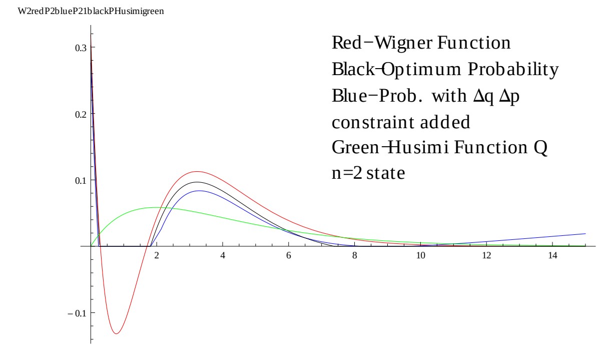

FIG. 2: The same plots as in Fig.1 for the n=2 coherent state . The optimum and Husimi distributions have $\sigma^2 = 0.268084$, and 0.64429 respectively.

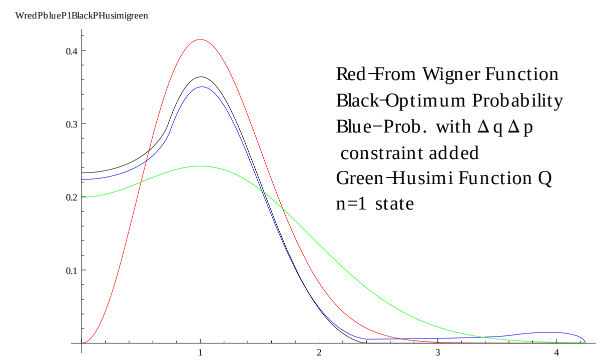

FIG. 3: For the n=1 coherent state , the position probabilities calculated from the optimum joint probabilities are seen to be closer to the true probability (given by the Wigner distribution) than the Husimi distribution result.

phase space densities reproducing two marginals of W, viz. quantum probability densities of $\vec{q}$ and $\vec{p}$. In $2N$-dimensional phase space, with $N \geq 2$, Roy and Singh [9] noted that in fact $N + 1$ marginals of W (e.g. for $N = 2$, probability densities of $(q_1, q_2), (p_1, q_2), (p_1, p_2)$) can be reproduced with positive densities; they conjectured that no more than $N + 1$ marginals can be so reproduced for arbitrary quantum states, the "$N + 1$" marginal theorem. This was proved later using an extension of Bell inequalities [10] to phase space by Auberson et al[11], who also derived the most general positive phase space density reproducing $N+1$ marginals; that density is non-unique since it contains an abitrarily specifiable phase space function. Among the continuous infinity of positive phase space densities reproducing $N+1$ marginals which one is closest to the Wigner Function ? Our method gives a straight forward answer; we give the variational answer explicitly for $N = 2$, and indicate briefly the generalization to $N \geq 2$. Find the phase space density $P(q,p)$ obeying positivity, minimum mean square fractional deviation from the Wigner distribution , reproducing the quantum probability densities of q, and p . Vary $P(q,p)$

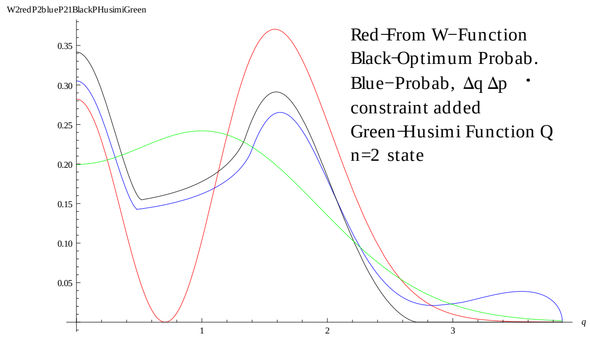

FIG. 4: Same plots as in Fig.3, for the n=2 coherent state of the oscillator.

to minimise the Lagrangian,

$$L = \int [(P - W)^2 + (2\lambda(q) + 2\mu(p))(P - W)]dqdp, \quad (24)$$

subject to the constraints,

$$\int (P - W)dp = 0, \int (P - W)dq = 0, \ P(\vec{q}, \vec{p}) \geq 0. \quad (25)$$

L is minimised if we choose for P, the function P_0 that makes L stationary whenever P_0 is positive, and zero otherwise:

$$P_{min} = P_0\theta(P_0), \ P_0 \equiv W - \lambda(q) - \mu(p), \quad (26)$$

where the multipliers $\lambda(q), \mu(p)$ are determined from the constraints. As in Sec. 2, we prove by direct subtraction that $L - L_{min} \geq 0$, the only change being the new choice of $P_0 \equiv W - \lambda(q) - \mu(p)$. The constraints yield a pair of coupled integral equations to determine $\lambda(q), \mu(p)$:

$$\int_{P_0 \geq 0} (\lambda(q) + \mu(p))dp = -\int_{P_0 \leq 0} W(q,p)dp,$$
$$\int_{P_0 \geq 0} (\lambda(q) + \mu(p))dq = -\int_{P_0 \leq 0} W(q,p)dq \ , \quad (27)$$

which complete evaluation of the optimum phase space density.For $N \geq 2$, the positivity constraint is supplemented by $N + 1$ marginal constraints, which can, for example, be chosen to be the series of probability densities of $(q_1, q_2, ..q_n), (p_1, q_2, ..q_n), ..(p_1, p_2, ..p_n)$, in which each member is obtained by replacing in the previous set one co-rdinate by its conjugate momentum.The optimal phase space density is again constructed by a Lagrange multiplier method which will now involve $N+1$ Lagrange multiplier functions.

6. Conclusion. We have proposed a general method to find the positive phase space distribution closest to the Wigner distribution that can be used in quantum optics as well as in time frequency analysis. A measure of quantumness emerges. Qualitative and quantitative improvement with respect to the Husimi function is seen explicitly; e.g. for the generalized coherent states, the optimum and Husimi distributions have respectively, for $n = 1$, $\sigma^2 = .277049$, and 0.509259, for $n = 2$, $\sigma^2 = 0.268084$, and 0.64429 . Similar improvements are expected in time frequency analysis.In $2N$-dimensional phase space the optimum positive density reproducing $N + 1$ marginals can be evaluated.

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